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Evaluation Of Methods For The Estimation Of Tributary Mass Loading Rates

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TECHNICAL REPORT NUMBER 187

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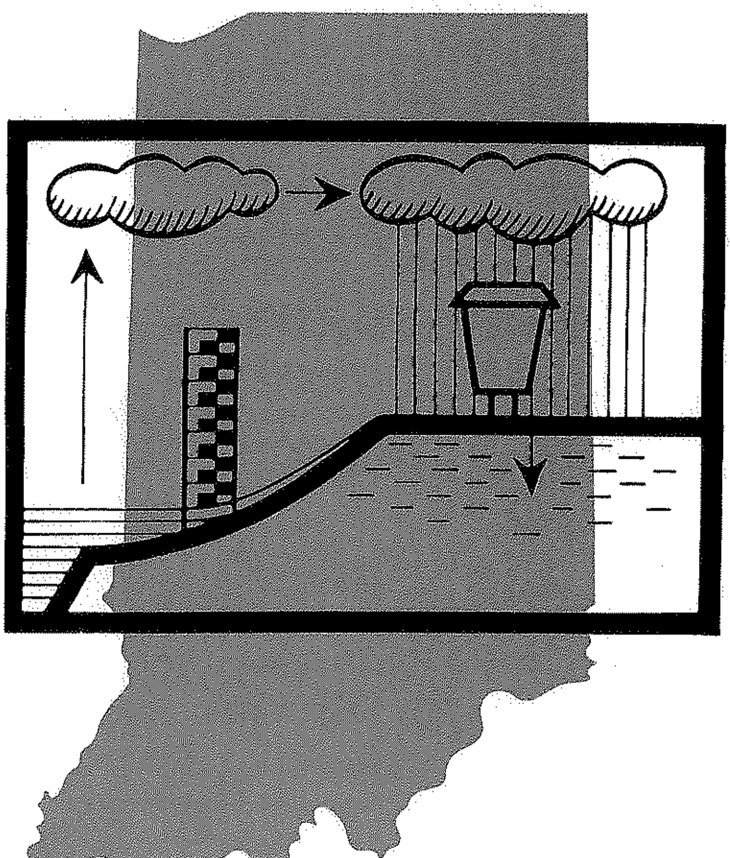

by

Stephen D. Preston
Victor J. Bierman, Jr.
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June 1989

PURDUE UNIVERSITY
WATER RESOURCES RESEARCH CENTER
WEST LAFAYETTE, INDIANA

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ASTRACT

Tributary loading estimation methods were evaluated for application to a range of tributary types including highly event responsive systems. Evaluations were performed by conducting retrospective studies with comprehensive sets of field data for flow rates and total phosphorus concentrations. Four estimators from three broad categories were selected for study based on their performance in previous research. Estimators were evaluated using Monte Carlo sampling studies in which random subsamples of complete loading records were used to estimate annual mass loads. These estimates were then compared to "true" loads determined by calculations using the entire record. Beale's Ratio Estimator consistently provided unbiased estimates, although stratification was necessary under event sampling. Differences in hydrograph characteristics played a strong role in the overall level of estimate error and in the amount of bias in averaging and regression estimators. Characteristics that are hypothetically responsible for the level of estimate error in different tributaries include frequency, magnitude and duration of high flow events. Sensitivity studies are currently underway to determine which of these characteristics introduce the greatest error. Daily flow simulation models to be used in sensitivity studies are described.

1. JUSTIFICATION OF WORK PERFORMED

1.1 Introduction

Impacts of contaminants on water bodies must be assessed within a quantitative framework in order to provide a basis for regulation in the form of wasteload allocations (U.S. Environmental Protection Agency, 1985). An essential component of this framework is the mass balance of contaminants between inputs and spatial / temporal distributions in the water body. Mass balances cannot be conducted unless there are useful and scientifically valid methods for estimating loading rates of contaminants from tributary sources.

Currently available statistical load estimators have been evaluated for application to Great Lakes tributaries (Dolan et al., 1981; Heidtke et al., 1986). However, these evaluations have been based on a small number of tributaries and a limited range of hydrologic conditions. Differences in system hydrology are known to affect load estimation (Richards and Holloway, 1987) and statistical estimators should be evaluated over the full range of tributary types.

This research involved the evaluation of statistical methods for estimating tributary loading rates of contaminants. Work reported here was performed during the second year of a two year project. During the first year, statistical loading estimators were evaluated for application to a range of contaminant types. Work during the second year emphasizes the evaluation of estimator performance when applied over a range of hydrologic conditions.

Results from the present research can be used directly in the application of models for contaminant mass balances and waste load allocations for inland lakes, nearshore embayments and the Great Lakes. They can be used to conduct retrospective studies with existing data or to design sampling programs for new studies.

1.2 Problem Definition

Tributary contaminant loading is a continuous process that can be represented as the product of flow and concentration over time. In mathematical terms loading can be described by:

$$L = \int_0^T C\,Q\;dt$$

Where

L = load (mass transported over period T)

C = concentration (mass/volume)

Q = flow (volume/time)

In practice, flow can be measured continuously and inexpensively using automated stage recorders and stage - discharge relationships. However, concentration for most water quality constituents can only be measured at discrete locations in time, and often at much lower frequencies than flow rates. Thus tributary loads must be estimated from a finite number of data points, e.g.

$$L = \sum_{j=1}^{T/\Delta t} C_j\,Q_j\;\Delta t$$

Error can be minimized by collecting a large number of samples. However, concentration measurements are expensive and a practical balance must be maintained between an acceptable level of error and cost. Consequently, accuracy and precision of tributary load estimates are limited by the number of available concentration data.

An efficient sampling program and statistical estimation technique can substantially improve the accuracy of the load estimate. A wide variety of approaches have been proposed for load estimation. However, no clear criteria for sampling design or choice of statistical estimation method have been defined. Results from existing studies of load estimation techniques are often conflicting because test conditions have been limited.

Loads cannot be known accurately without direct measurement of concentration close to the point of discharge. Point sources of contaminants can be measured accurately; however, diffuse sources within the watershed are difficult to measure. Deterministic watershed loading models have been developed. However, they are so complex and data intensive that it is sometimes impossible to even evaluate their performance (e.g. Leytham and Johanson, 1979).

An obstacle to the interpretation of available data for contaminants is that hydrologic differences among tributaries affect loading estimation. Differences in system hydrology may impact estimator performance in two ways. First, highly event responsive systems react quickly to the onset of storms and subsequently recede rapidly. These short term events have a low probability of being sampled and this may cause an underestimation of load. A second potential impact is that event responsive systems may exhibit different constituent behavior than less responsive systems. For example, rapid event response may change constituent concentrations by elevating non - point source loads, by resuspending sediments or by dilution. In contrast, constituent concentrations in unresponsive systems may have a weak or non - existent relationship to the flow rate. To assess the effect of these impacts load estimation methods should be evaluated over a full range of hydrologic conditions.

1.3 Scope

This research has involved the evaluation of tributary load estimation methods under a range of conditions. Results are presented for the second year of work on a two year project. Work performed during the first year emphasized load estimation of a variety of contaminant types and the utilization of suspended solids as an auxiliary variable. Work performed during the second year emphasized load estimation over a range of hydrologic conditions.

A portion of the work presented here consisted of retrospective studies using known comprehensive data bases. The use of the Grand River (1976/77) data base was originally proposed for the second year. However, this work was accelerated and results were presented in the final technical report for the first year (Bierman et al., 1988). In place of the Grand River, three Ohio tributary data sets (Hickory Creek, Maumee River and Sandusky River) were obtained and were used for a more comprehensive evaluation of estimator performance over a broader range of hydrologic conditions. Results from the Ohio tributaries were then compared to results from the first year (Grand and Saginaw Rivers, Michigan). Total phosphorus was used in all evaluations because it is the one constituent that is common to all of the tributary test cases.

Work performed during the second year also included the design of methods for simulation of flow and concentration data. Simulation will allow the evaluation of estimation methods over a wider range of conditions and thus expand the scope of study. Development of methods that accurately reproduce hydrograph and chemograph characteristics is still in progress and is concentrating on daily flow simulation. Two daily flow simulation models are being evaluated.

As in the first year estimators have been evaluated using Monte Carlo sampling studies. Complete loading records were subsampled under typical sampling scenarios and then compared to "true" loadings determined from the entire record. Based on work performed during the first year the number of estimation approaches was reduced to only the most promising methods.

1.4 Objectives

The objectives of research conducted during the second year were the following:

1. Evaluate the most promising tributary load estimators when used for the estimation of total phosphorus loads in three Ohio tributaries.
2. Compare performance of loading estimation methods over the range of hydrologic types represented by the Michigan and Ohio tributaries.
3. Develop methods for the simulation of loading data.

2. LITERATURE REVIEW

2.1 Estimation Approaches

Estimation approaches can be grouped into three main categories including averaging, ratio and regression estimators. Averaging estimators are the simplest approach and have been commonly applied for lack of better techniques. Ratio estimators have been adapted to the loading problem from the statistical literature (Cochran, 1977) and have performed well in evaluation studies (Dolan et al., 1981). Regression estimators or "rating curves" have been used to estimate loading rates of many constituents, particularly suspended solids (Walling, 1977). Details of these statistical estimators have been described elsewhere (Bierman et al., 1988). A summary of this information is presented below.

Averaging estimates are made by using averages as representative measures of flow, concentration or load for a given time interval and summing over the year. These estimators are flexible and easy to apply. However, implicit assumptions such as independent and identically distributed data are rarely met. Violations of assumptions may lead to estimation bias especially if the sampling program does not collect data from the entire range of flow and concentration (Dolan et al., 1981; Ferguson, 1987).

Ratio estimators have been adapted from Survey Sampling statistics for application to the load problem. This approach uses flow data as the auxiliary variable and load as the dependent variable. The ratio estimator is considered a "Best Linear Unbiased Estimator" (BLUE) under two conditions (Cochran, 1977):

1. The relation between y_i and x_i is a straight line through the origin
2. The variance of y_i about this line is proportional to x_i

where y_i is the dependent variable and x_i is the auxiliary variable. These conditions are commonly observed in the relationship between load and flow, and Beale's ratio estimator has been used successfully to estimate loading rates of total phosphorus (Dolan et al., 1981).

Regression methods (rating curves) have traditionally been applied for estimating tributary loads of suspended solids and other constituents (Walling, 1977). Generally log - log regressions are applied because flow and concentration are assumed to be described by a bivariate lognormal distribution. Log - log relationships are theoretically biased when used for prediction purposes and Ferguson (1986) demonstrated that accuracy of log - log regressions can be improved by using a bias correction factor. Cohn et al. (1989) improved the bias correction factor to yield a minimum variance unbiased estimator (MVUE) for log - log relationships.

Stratification is a modification of all of the above approaches that can substantially improve estimate accuracy and precision (Richards and Holloway, 1987). Stratification is performed by dividing the population into homogeneous subunits called strata. Subunits can be sampled separately and the estimates combined to obtain an estimate over the entire population. This allows allocation of samples to individual strata based on the level of stratum variability.

Estimator performance is often dependent upon the sampling program under which data were collected. Sampling should be performed in a manner that insures collection of data from the entire range of flow and concentration. Under systematic sampling programs short term flow events can be missed leading to underestimation of tributary load (Yaksich and Verhoff, 1983). This can be avoided by specifically sampling events and stratifying data into event and non - event categories (Richards and Holloway, 1987). Flow stratification has been shown to reduce estimate error (Heidtke et al., 1986; Preston et al., 1989); however, the separation between event and non - event flows is difficult to determine objectively.

2.2 Estimator Evaluations

Empirical studies have been carried out to compare estimation approaches. Dolan et al. (1981) compared ten estimation methods as applied to total phosphorus loads in the Grand River. Beale's stratified ratio estimator provided estimates with the lowest error under random sampling. Heidtke et al. (1986) compared two ratio and four regression estimators under seven sampling strategies. Beale's stratified ratio estimator provided consistent low bias in total phosphorus load estimates. However, none of the estimators consistently provided the lowest mean square error. Ferguson (1987) compared five estimation methods using suspended solids loads and found the bias corrected rating curve to yield the lowest error.

During the first year of this study estimators was compared using data for a variety of contaminants (Bierman et al., 1988). A total of 24 estimators were compared under semi - monthly and monthly + event sampling strategies. No one group of estimators (averaging, ratio or regression) was clearly superior for all test cases. However, individual estimators within each group consistently provided low error estimates. Ratio estimators were more robust than other estimators to bias caused by strong short term events. Test case characteristics such as the number and magnitude of flow events and the type of flow - concentration relationship appeared to have a strong impact on estimator performance.

The effects of events can be reduced by event sampling and stratification. Research has been performed to investigate methods of designing sampling programs for this purpose. Heidtke et al. (1986) and Richards and Holloway (1987) have investigated stratification methods for loading estimation. Definition of strata cutpoints and sample allocation within strata were investigated.

Research has also been performed to classify tributaries based on their hydrologic characteristics. An optimal classification scheme may provide a basis for choosing sampling and estimation approaches. Richards (1988) investigated tributary classification criteria based on system variability. Data analysis of tributary flow records led to a four - level classification scheme that was based on the responsiveness of the system to events. In order of most to least responsive, the categories are "Event Responsive", "Variably Responsive", "Stable" and "Superstable".

3. METHODS

3.1 Estimation Approaches

Based on results from work in the previous year, a reduced set of estimation approaches was chosen for study. Estimators that clearly did not perform well were eliminated. In addition, only one estimator was chosen from a particular group if no significant differences in performance were observed. Chosen estimators are listed in Table 1. Reasons for these choices are discussed below.

Of averaging estimators only one consistently provided low error estimates (Preston et al., 1989). Method 1 in Bierman et al. (1988) uses daily flow with monthly average concentration. This estimator provided accurate and precise estimates for many of the test cases considered. Other averaging estimators provided estimates that were biased or imprecise or both. Thus Method 1 was the only averaging method retained for study in the second year.

Little difference was observed among ratio estimators under similar non - event sampling scenarios (Bierman et al., 1988). The simple ratio estimator was slightly more precise in most cases and the estimator of Hartley and Ross (1954) was slightly less precise. However, these differences were small and were not consistent among test cases. Beale's ratio estimator has been used most commonly for load estimation. Since other ratio estimators did not perform significantly better than Beale's, they were dropped from consideration.

Only one of the regression estimators evaluated by Bierman et al. (1988) and Preston et al. (1989) was chosen for further study. The robust regression described by Watson (1985) provided estimates with large errors in many cases and was dropped. Cohn et al. (1989) described an improved method of compensating for bias in the log transformed rating curve. The minimum variance unbiased estimator (MVUE) described by Cohn et al. (1989) was applied to the Grand and Saginaw test cases (Preston et al., 1989). The MVUE produced estimates with less error than the estimator of Ferguson

TABLE 1. MATHEMATICAL DESCRIPTION OF TRIBUTARY LOAD ESTIMATION METHODS

METHOD TYPE	MATHEMATICAL EXPRESSION	REFERENCE
Averaging	$\hat{L} = \sum_{h=1}^{12} \sum_{j=1}^{N_h} q_{jh} \left(\sum_{i=1}^{n_h} \frac{c_{ijh}}{n_h} \right)$	Dolan et al. (1981)
Ratio	$\hat{L} = Q \left(\frac{\bar{l}}{\bar{q}} \right) \left[\frac{1 + \left[\frac{(1-f)}{n}\right] \left[\frac{S_{lq}}{(\bar{l})(\bar{q})}\right]}{1 + \left[\frac{(1-f)}{n}\right] \left[\frac{S_q^2}{(\bar{q}^2)}\right]} \right]$	Beale (1962)
Regression	$\hat{L} = \sum_{i=1}^{n} q_i c_i + \sum_{j=1}^{N-n} q_i \left[\exp (\hat{\beta}_0 + \hat{\beta}_1 \ln q_i) \right] [\text{MVUE BCF}]^{\dagger}$	Cohn et al. (1989)

† MVUE Bias correction factor - see Cohn et al. (1989).

(1986) and was therefore retained for future study.

Stratification was performed only for Beale's Ratio estimator. As was performed in Bierman et al. (1988), data were separated into event and non - event flows based on the hydrographs of the particular tributary.

3.2 Evaluation Criteria

In both the first and second year of work, estimation methods were evaluated using Monte Carlo sampling studies. Complete records of daily flow and concentration values for each test case were randomly subsampled under specified sampling scenarios. Subsamples were then used to estimate total tributary load using each estimator. Repetition of this process (n=1000) yielded estimate distributions that provide information on the potential error of a given estimator - sampling scenario combination.

Complete records were subsampled under systematic and event sampling. Systematic sampling is commonly performed to estimate tributary load and this was conducted at a semi - monthly frequency. Systematic sampling was performed by randomly selecting daily flow and concentration values within time periods defined by the frequency. For example, monthly sampling was performed by randomly choosing values within each month using a uniform random deviate generated by the algorithm of Ang and Tang (1984). Event sampling was performed in a similar manner and consisted of monthly samples plus 12 high flow samples randomly chosen from throughout the year. Semi - monthly and event sampling are presented here because they both consist of 24 samples and are comparable on that basis.

Estimate distributions were compared on the basis of mean square error (MSE):

$$MSE(\hat{\mu}) = E(\hat{\mu} - \mu)^2$$

where

$\hat{\mu}$ = individual estimate

μ = known true value

This quantity can be further broken down into bias and variance. Bias represents the difference between the average estimate and the true value. Variance is a measure of the spread of the estimate. These measures can be derived from the MSE:

$$\mathrm{MSE}(\hat{\mu}) = E\left[(\hat{\mu} - \bar{\hat{\mu}}) + (\bar{\hat{\mu}} - \mu) \right]^2$$

where

$$\bar{\hat{\mu}} = \text{mean estimate.}$$

This equation can be expanded to

$$\mathrm{MSE}(\hat{\mu}) = E(\hat{\mu} - \bar{\hat{\mu}})^2 + 2(\bar{\hat{\mu}} - \mu)E(\hat{\mu} - \bar{\hat{\mu}}) + (\bar{\hat{\mu}} - \mu)^2.$$

Since $E(\hat{\mu} - \bar{\hat{\mu}}) = 0$

$$\mathrm{MSE}(\hat{\mu}) = \text{variance of } \hat{\mu} + (\text{bias})^2.$$

Optimally an estimator should be precise (low variance). Precision is defined here as the inverse of the standard error of the estimate. Standard error is defined by

$$SE = \left[\frac{\sum_{i=1}^{n} (\hat{\mu} - \bar{\hat{\mu}})^2}{n-1} \right]^{1/2}$$

The estimator should also be accurate (low bias) and this is quantified by the difference between the mean estimate and the true value. To allow comparison over all test cases, units of estimated bias and standard error are normalized as percent of the "true" value. The normalized MSE is calculated as the sum of the normalized bias squared and the normalized standard error squared.

The actual true mass load cannot be determined exactly without a continuous record of flow and concentration. Hence, only a high frequency approximation is possible. Daily values of flow and concentration represent a much higher frequency than most sampling programs (e.g. - monthly, semi - monthly). Thus the actual true values as used in this paper are approximated as the sum of the products of flow and concentration using all available data for each test case.

3.3 Test Case Descriptions

High frequency data records were obtained from three tributaries located in the State of Ohio. The Maumee and Sandusky Rivers are located in northern Ohio and discharge to Lake Erie. Hickory Creek is a tributary of the Sandusky River and was included because of its smaller size and rapid response to events. High frequency measurements (1 - 4 /day) of flow and concentration were collected by the water quality laboratory of Heidelberg College in a project sponsored by the Great Lakes National Program Office of the U.S. Environmental Protection Agency (Baker, 1988). Data were obtained from Heidelberg College for the period 1976 - 1986. However, only three years (1983 - 1985) were chosen for study because of their relatively complete records.

These tributaries were chosen for study because they have substantially different flow characteristics than previously studied Michigan tributaries. Strong differences in event frequencies and flow - concentration relationships are expected between the Michigan and Ohio tributaries. In a tributary classification study, the Ohio streams were categorized among the most responsive of Great Lakes tributaries (Richards, 1988). In the same study the Michigan tributaries were placed in the "Stable" category.

Data from the Ohio tributaries were treated in a manner similar to the Michigan data. Sampling studies were performed on a daily basis and values from a specific time of day were taken as representative. Data were available for most days in each tributary year (Table 2). However, short gaps were interpolated using time series models and thus records are partially synthetic.

3.4 Preliminary Data Analysis

Initial data analyses were carried out to characterize tributary flow and concentration records. Results of these analyses provide a basis for interpretation of sampling study results and allow the development of hypotheses concerning the causes of estimate error in a given tributary. These hypotheses can then be tested using data simulation studies. A description of data analysis results and test case characteristics follows.

TABLE 2. TEST CASE SUMMARIES INCLUDING FRACTION OF RECORD THAT ARE ACTUAL MEASUREMENTS (n/N) AND ESTIMATED "TRUE" ANNUAL LOADS

TRIBUTARY	YEAR	n/N	TRUE LOAD (MT)
Grand River (MI)	1976/77	361/365	634.
Saginaw River (MI)	1978	219/365	617.
Saginaw River (MI)	1980	247/365	462.
Hickory Creek (OH)	1983	352/365	41.
Hickory Creek (OH)	1984	364/366	53.
Hickory Creek (OH)	1985	343/365	43.
Maumee River (OH)	1983	365/365	2217.
Maumee River (OH)	1984	363/366	2244.
Maumee River (OH)	1985	318/365	2749.
Sandusky River (OH)	1983	334/365	389.
Sandusky River (OH)	1984	325/366	639.
Sandusky River (OH)	1985	339/365	457.

Statistical summaries of test case total phosphorus concentration data are presented in Table 3. Mean total phosphorus concentrations were similar in most tributaries and ranged from approximately 0.14 to 0.26 mg/l. Concentrations were highest in the Maumee River which averaged approximately 0.25 mg/l. Concentrations were more variable in the Ohio tributaries as indicated by the higher standard deviations.

Strong differences in the flow characteristics of the streams are revealed by the statistical summaries presented in Table 4. Hickory Creek and the Sandusky River are smaller streams relative to the Michigan tributaries and this is reflected in the mean flow rate. Variability is much greater in the Ohio tributaries. Coefficients of variation ($s/\bar{x}$) range from 0.8 to 1.1 in the Michigan tributaries and from 1.5 to 2.5 in the Ohio tributaries. High flow variability in the Ohio tributaries is also indicated by the extreme range of flow rates especially in the Maumee River.

Hydrographs for the 12 tributary/year test cases are presented in Figures 1 - 4. Figure 1 illustrates the relatively sluggish response of the Michigan tributaries in which flow events can occur over a period of weeks. Hydrographs for the Ohio tributaries (Figures 2 - 4) illustrate rapid event responsiveness. Events in these systems are short in duration, can be characterized by rapid rises and recessions and can occur in high frequency. The highest flow events occurred in 1985 in all Ohio tributaries except the Sandusky which also had high flows in 1984. In all tributaries high flows occurred in greatest frequency in the early and late parts of the year.

Significant differences in the behavior of total phosphorus are apparent between the Michigan and Ohio tributaries. Figures 5 and 6 illustrate normalized flow and concentration for the Michigan tributary test cases and for the Ohio tributaries during 1983. Data are normalized to the same scale by subtracting the annual mean and dividing by the annual standard deviation. In general flow / concentration relationships in the Michigan tributaries are weak, although an approximate inverse relationship is observed in the Grand River

TABLE 3. STATISTICAL SUMMARY OF TOTAL PHOSPHORUS CONCENTRATION IN THE OHIO TRIBUTARIES DURING THE PERIOD 1983 TO 1985

TRIBUTARY	YEAR	MEAN (mg/l)	STANDARD DEVIATION	MINIMUM	MAXIMUM
Grand River (MI)	1976/77	0.193	0.105	0.060	1.72
Saginaw River (MI)	1978	0.189	0.066	0.068	0.659
Saginaw River (MI)	1980	0.138	0.047	0.058	0.467
Hickory Creek (OH)	1983	0.184	0.139	0.033	0.846
Hickory Creek (OH)	1984	0.194	0.152	0.055	1.019
Hickory Creek (OH)	1985	0.174	0.127	0.035	0.939
Sandusky River (OH)	1983	0.187	0.147	0.003	1.067
Sandusky River (OH)	1984	0.189	0.169	0.071	1.672
Sandusky River (OH)	1985	0.206	0.171	0.057	1.747
Maumee River (OH)	1983	0.259	0.158	0.081	0.969
Maumee River (OH)	1984	0.245	0.142	0.117	1.204
Maumee River (OH)	1985	0.257	0.186	0.030	1.490

TABLE 4. STATISTICAL SUMMARY OF FLOW DATA IN THE OHIO TRIBUTARIES DURING 1983 TO 1985

TRIBUTARY	YEAR	MEAN (cms)	STANDARD DEVIATION	MINIMUM	MAXIMUM
Grand River (MI)	1976/77	127.	142.	32.	833.
Saginaw River (MI)	1978	93.	143.	19.	847.
Saginaw River (MI)	1980	104.	85.	<1.	443.
Hickory Creek (OH)	1983	3.7	7.1	<1.	51.9
Hickory Creek (OH)	1984	4.3	10.1	<1.	73.4
Hickory Creek (OH)	1985	4.1	10.1	<1.	103.
Sandusky River (OH)	1983	32.	54.	<1.	306.
Sandusky River (OH)	1984	56.	113.	1.	708.
Sandusky River (OH)	1985	39.	70.	1.	542.
Maumee River (OH)	1983	159.	235.	2.	1360.
Maumee River (OH)	1984	160.	257.	1.	1368.
Maumee River (OH)	1985	190.	347.	4.	2538.

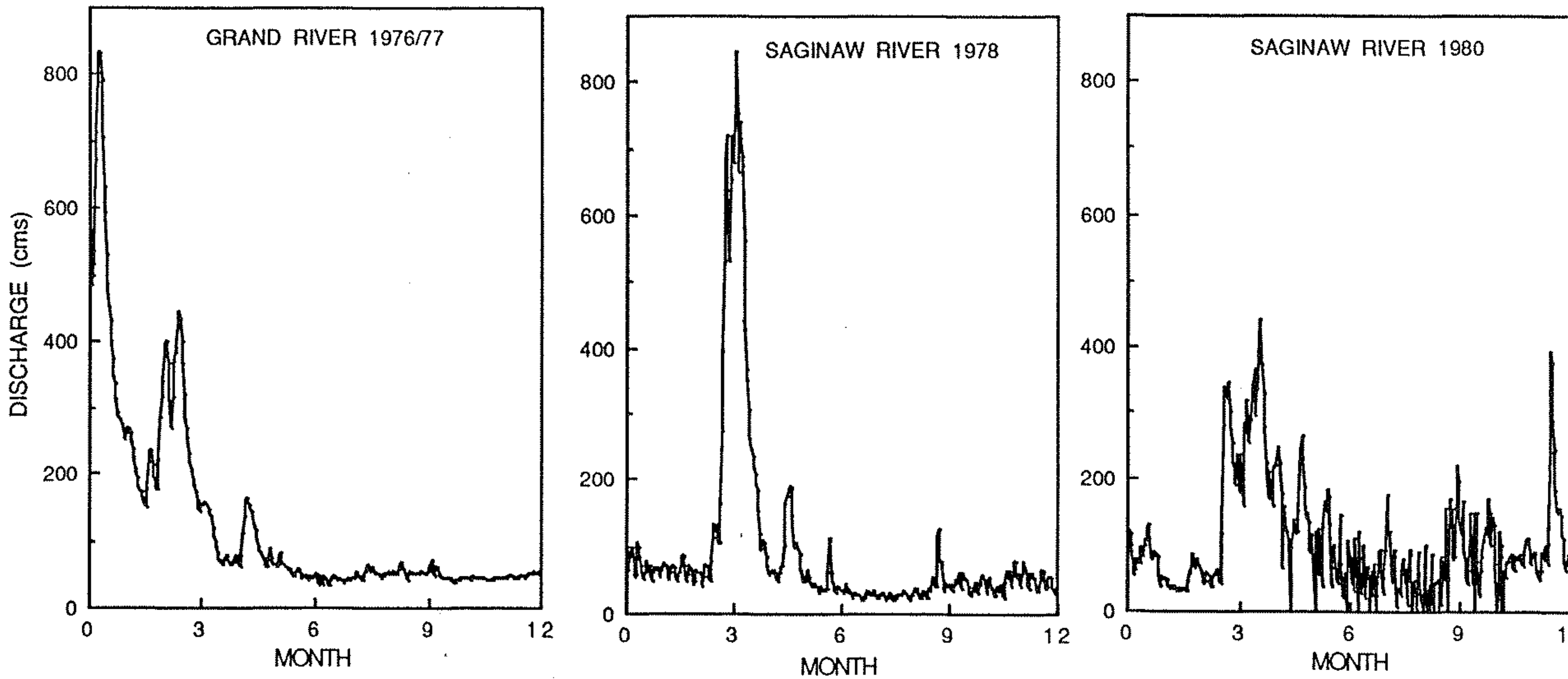

Figure 1. Annual hydrographs for the three Michigan tributary test cases.

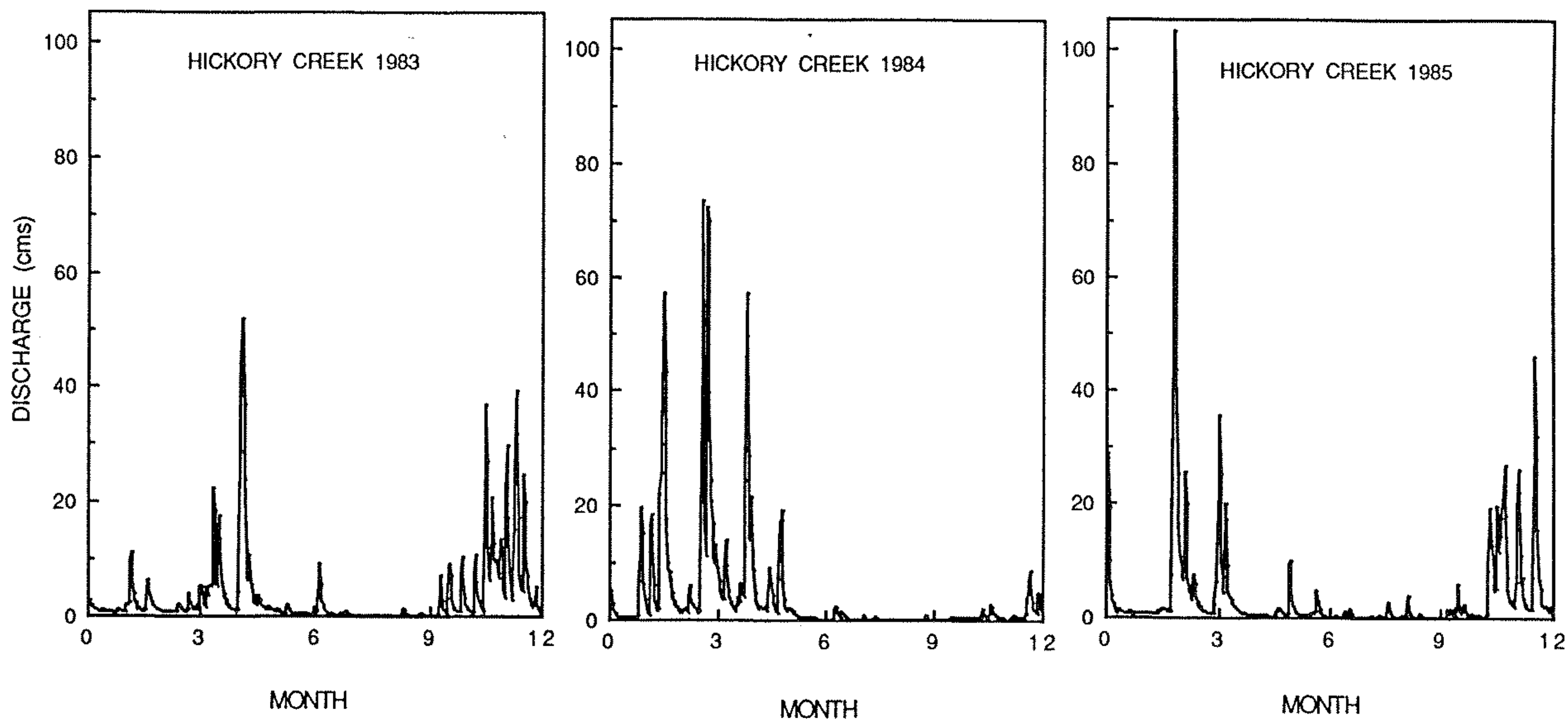

Figure 2. Annual hydrographs for Hickory Creek during 1983, 1984 and 1985.

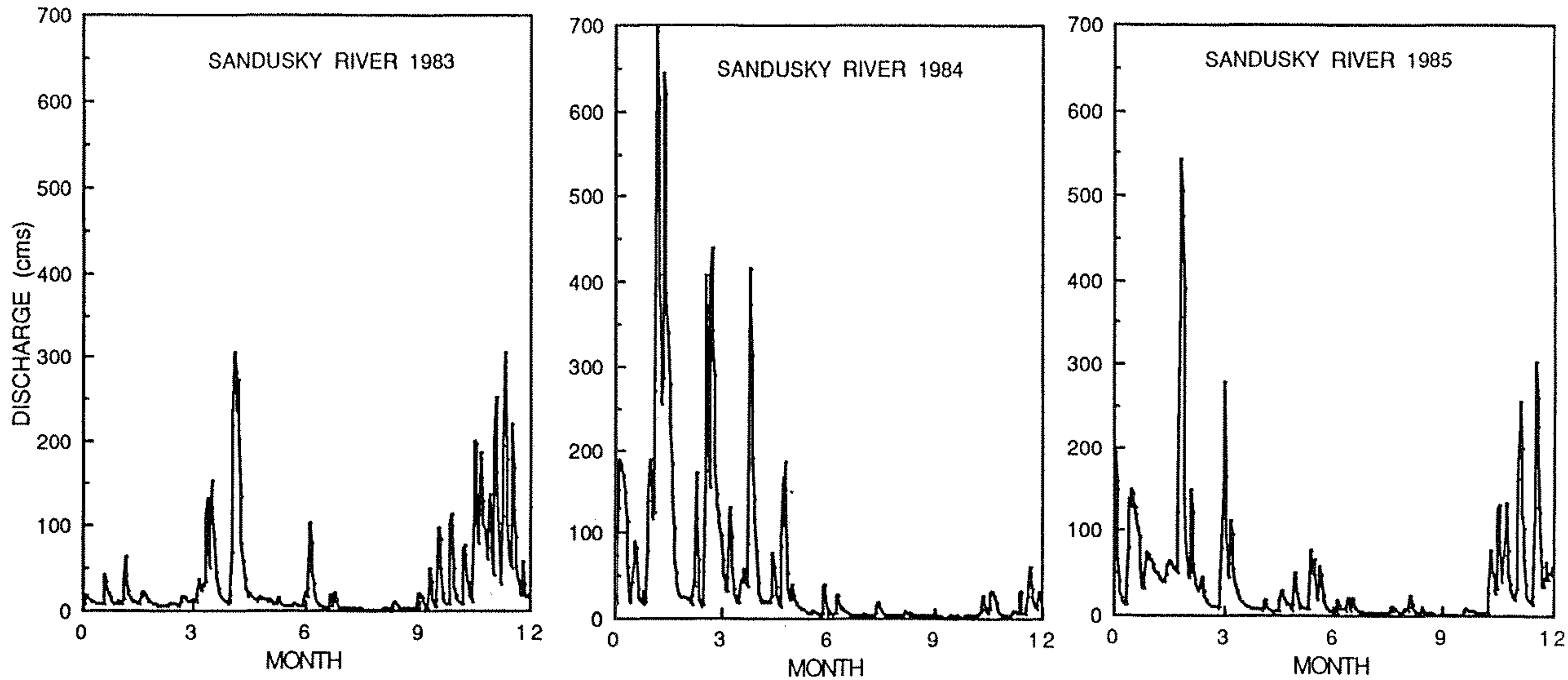

Figure 3. Annual hydrographs for the Sandusky River during 1983, 1984 and 1985.

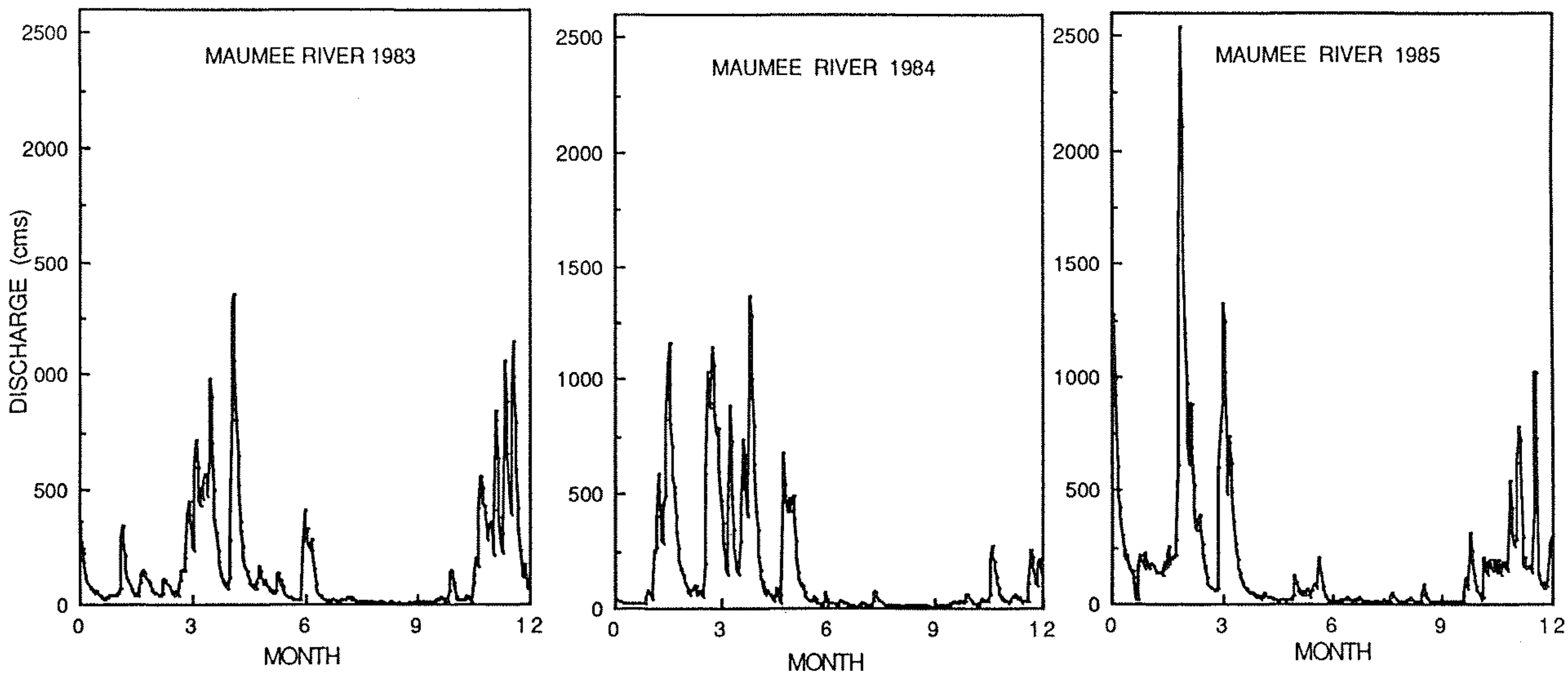

Figure 4. Annual hydrographs for the Maumee River during 1983, 1984 and 1985.

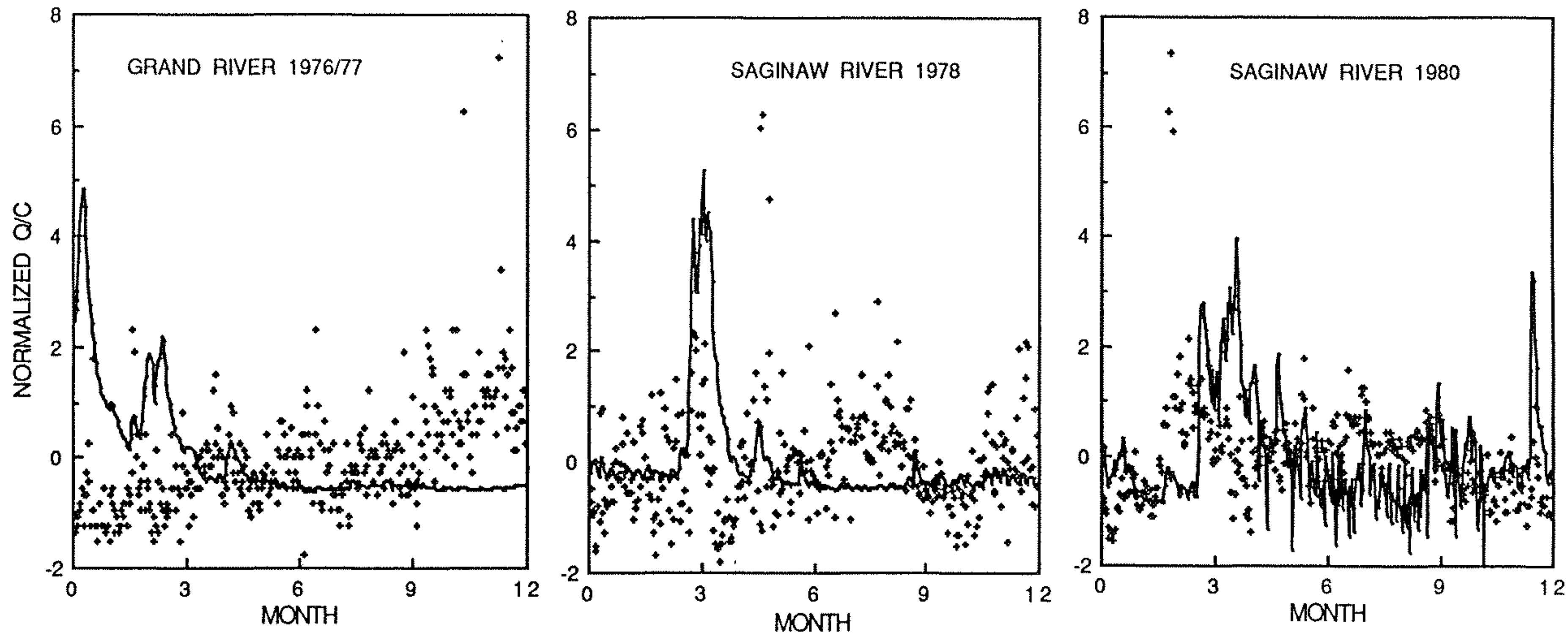

Figure 5. Normalized flow (solid line) and concentration (stars) for the Michigan tributary test cases. Data are normalized by subtracting the annual mean and dividing by the annual standard deviation.

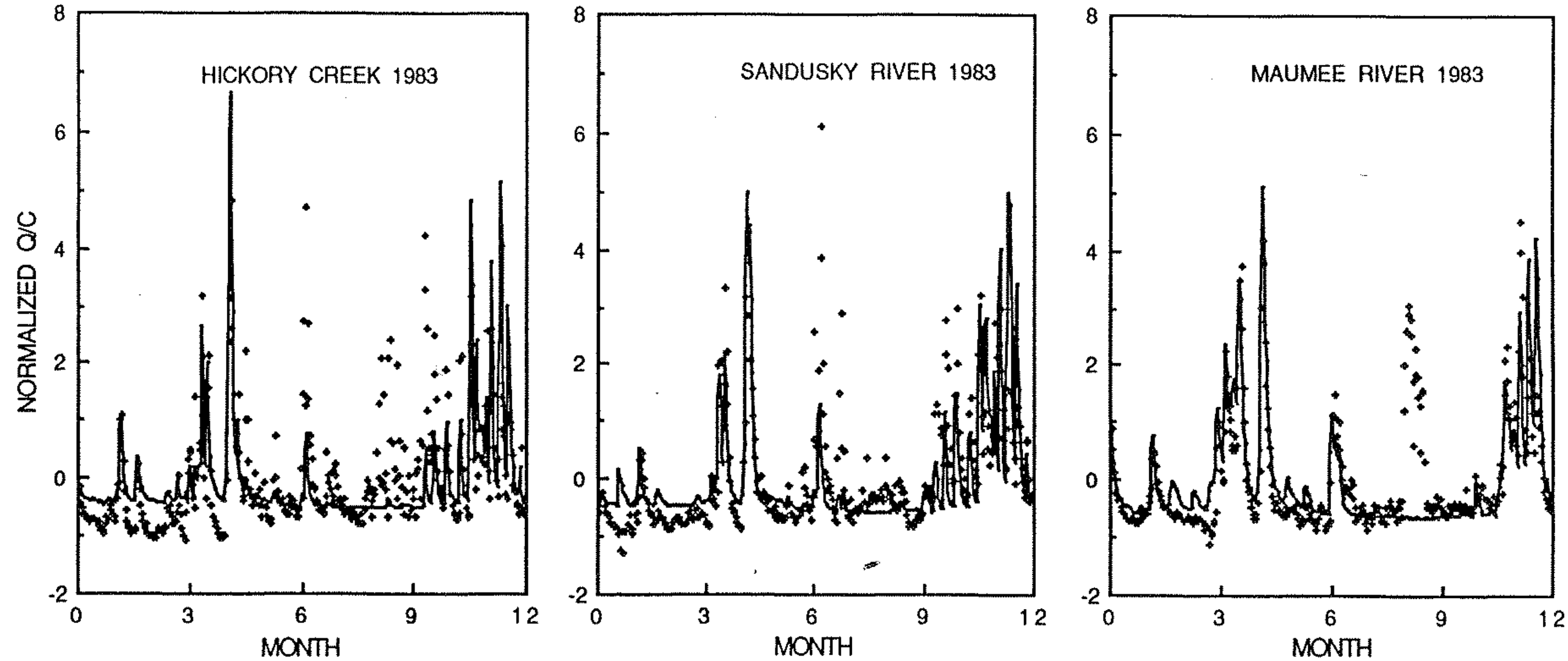

Figure 6. Normalized flow (solid line) and concentration (stars) for the Ohio tributary test cases during 1983. Data are normalized by subtracting the annual mean and dividing by the annual standard deviation.

(Figure 5). Total phosphorous concentration in the Grand is low during spring high flows and high during summer and fall low flows. In contrast a direct relationship is observed between flow and concentration in the Ohio tributaries (Figure 6). In all three Ohio tributaries phosphorus concentrations often increase with high flow events possibly due to resuspension or non - point source loading. An exception is observed in the Maumee River during the month of August.

These relationships can be further illustrated by plotting concentration vs. flow (Figures 7 and 8). Examination of concentration / flow plots provides an indication of how well specific estimators can be expected to perform. Strong exponentially increasing or decreasing relationships imply that regression estimators would perform well. In the Michigan tributaries, concentration remains relatively constant or decreases with increasing flow. This type of relationship has been attributed to dilution as a causal mechanism (Johnson, 1979) and is appropriate for the regression estimator. Figure 8 illustrates that the same relationships do not exist in the Ohio tributaries. In these systems concentration often increases in level and becomes more variable with high flow. This type of relationship has been attributed to flow driven release (Johnson, 1979) and its implications for load estimation are unclear.

Figures 9 and 10 illustrate the relationships between load and flow for the Michigan and Ohio (1983) tributaries respectively. In all cases a nearly linear relationship exists and variance in load increases with increasing flow. These are the two conditions under which the ratio estimator is a "Best Linear Unbiased Estimator" and the ratio estimator would therefore be expected to be unbiased in all systems. The linear relationship is observed because concentration values are weighted by flow to calculate load values. Thus even though differences in the flow / concentration relationship exist, the relationship between load and flow may consistently be linearly increasing. It is expected that the consistency of this relationship is one reason why the ratio estimator is robust to the bias observed in other estimators.

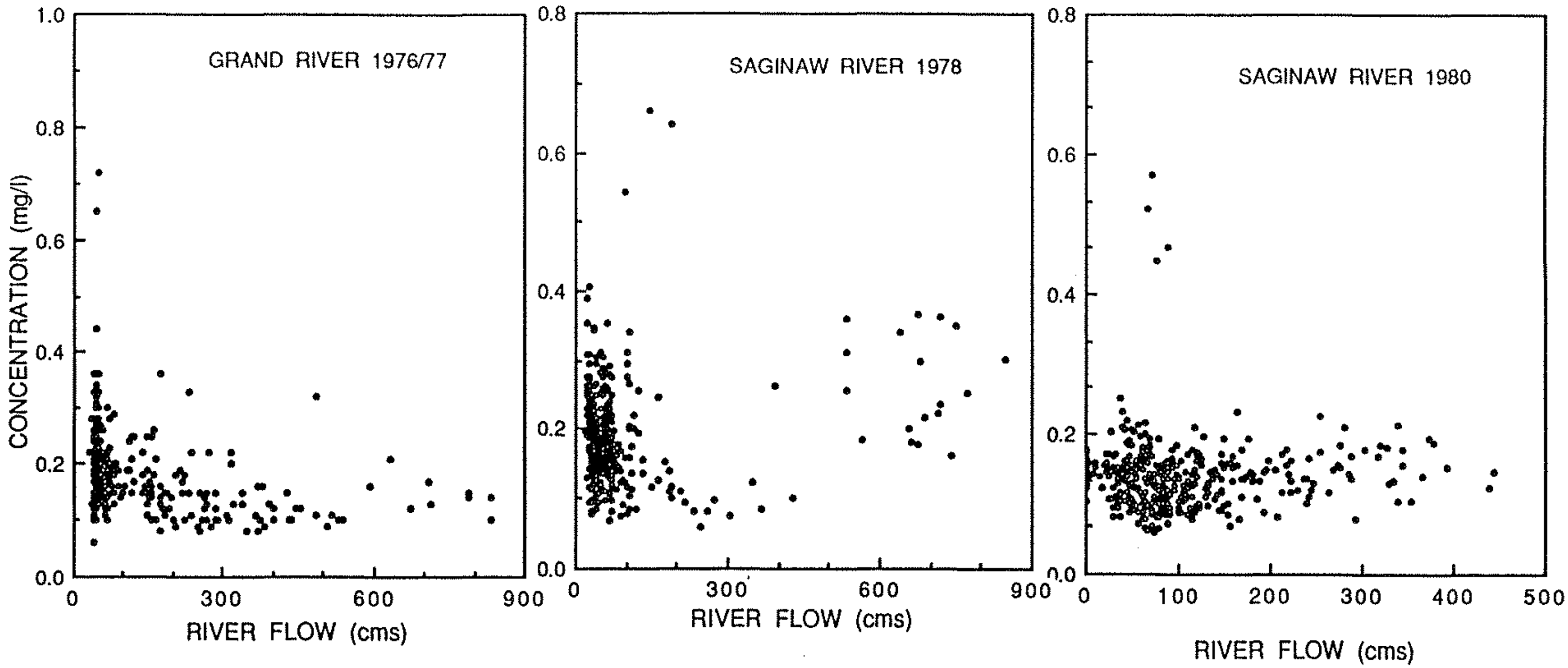

Figure 7. Relationships between flow and total phosphorus concentration in the Michigan tributaries.

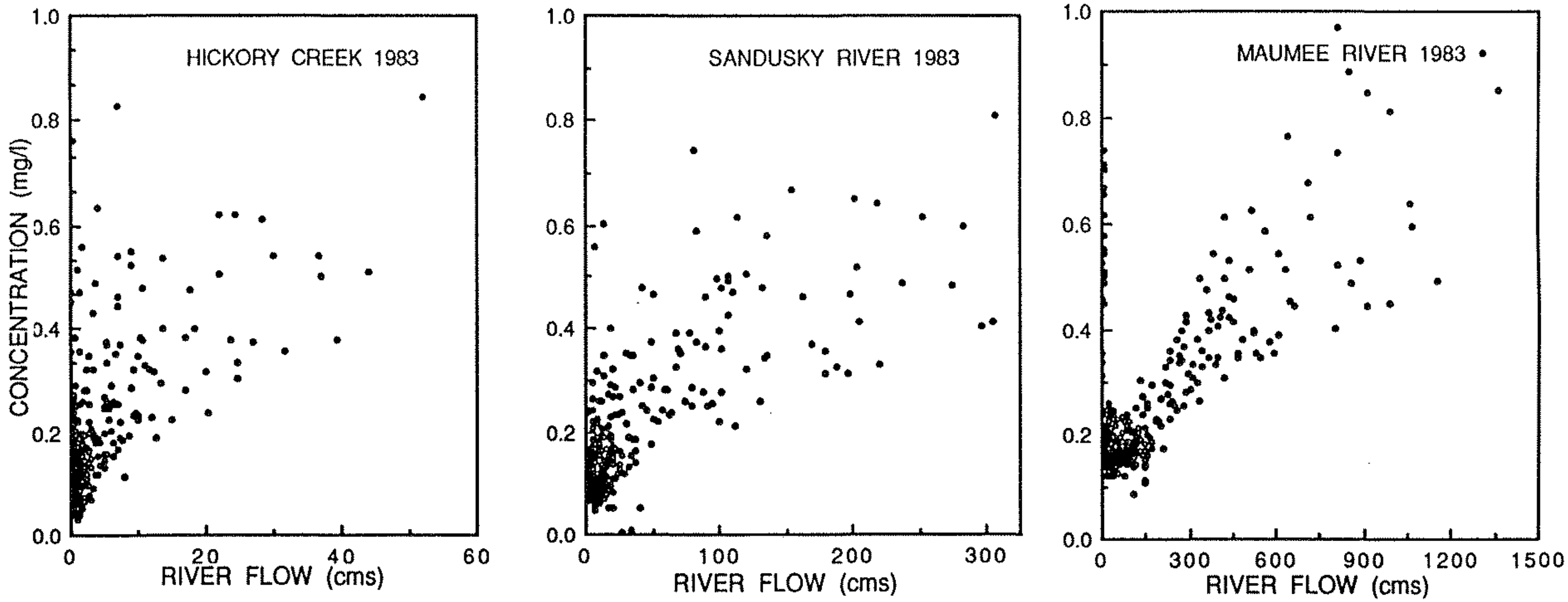

Figure 8. Relationships between flow and total phosphorus concentration in the Ohio tributaries during 1983.

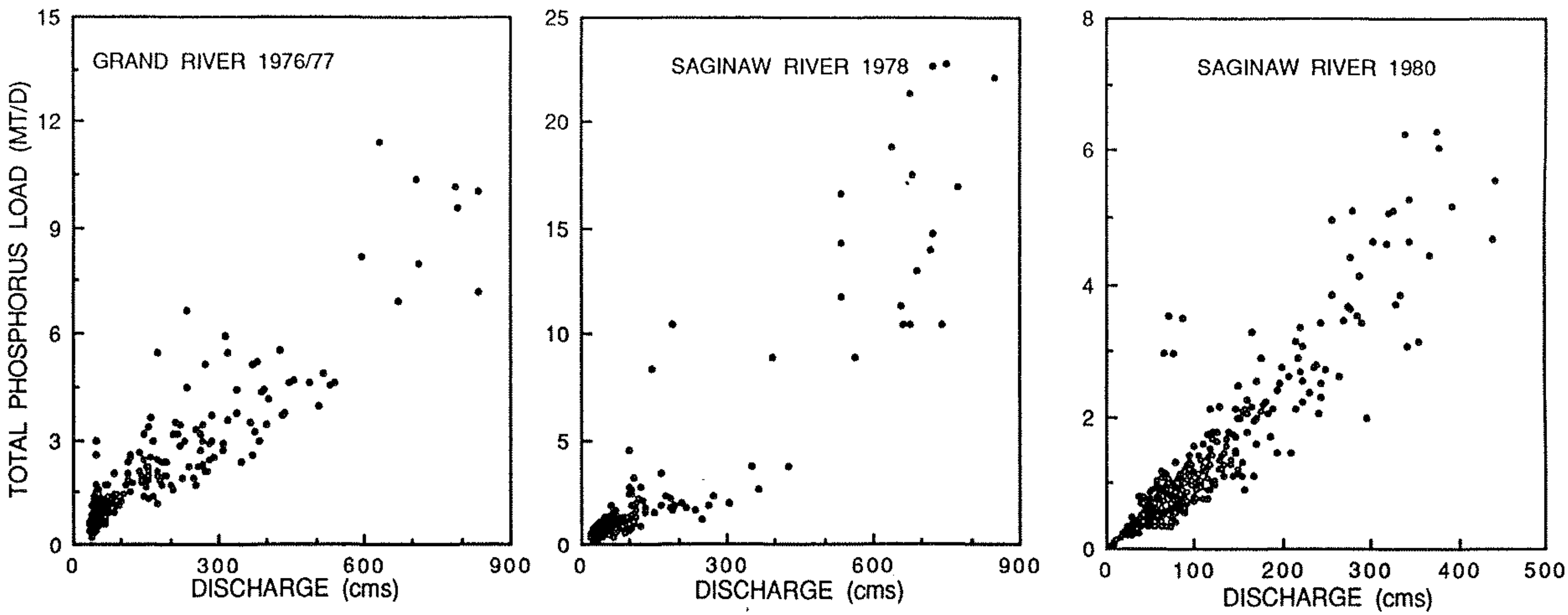

Figure 9. Relationships between flow and daily total phosphorus load in the Michigan tributaries.

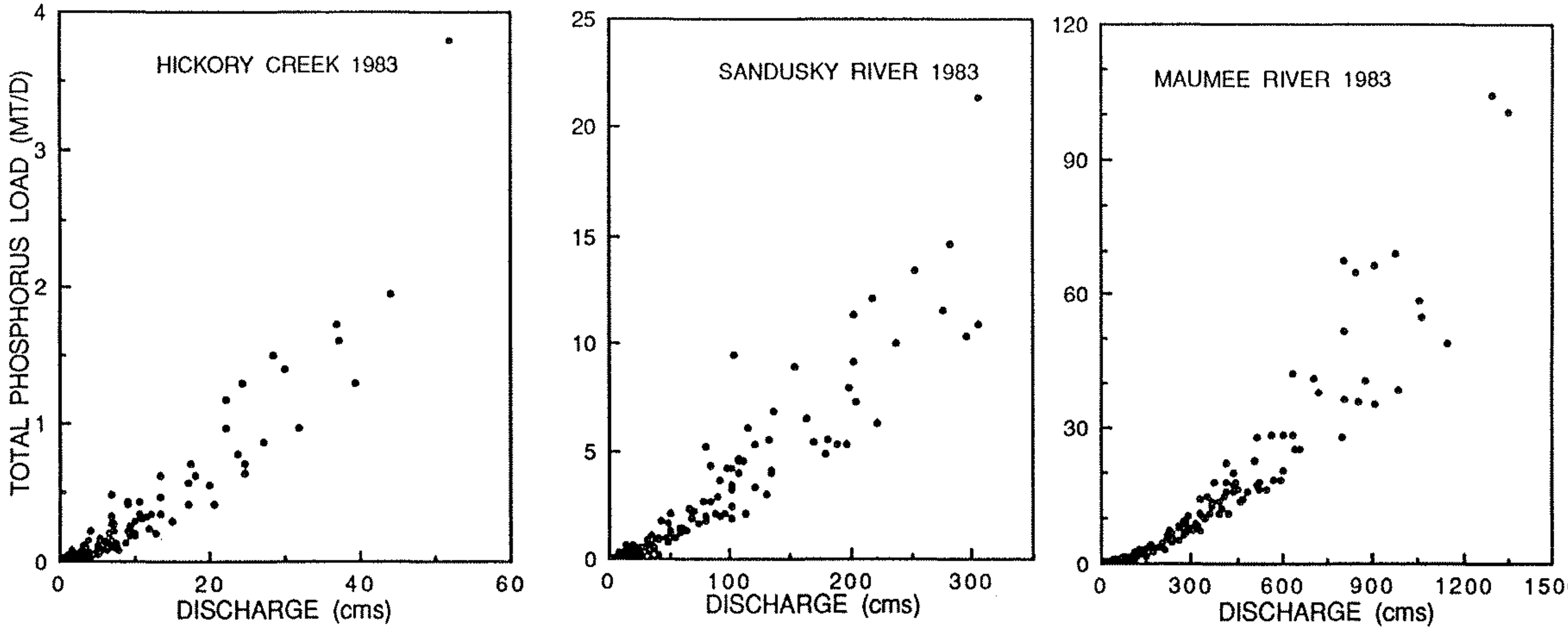

Figure 10. Relationships between flow and daily total phosphorus load in the Ohio tributaries during 1983.

4. RESULTS

4.1 Overview

Comparisons among the test cases are summarized in the form of bar charts (Figures 11 - 14). These figures present the MSE of each estimate distribution, but are subdivided into squared bias (open areas) and variance (hatched areas). To allow comparison over all test cases, units are normalized by dividing the bias and standard error by the "true" value. This converts all units to percent of true value and allows direct comparison. The Root Mean Square Error (RMSE) is the square root of the MSE and is referred to because it provides an indication of the expected percentage of error around a given estimate.

Results are grouped to allow a concise and understandable presentation. The Michigan tributary results for the four considered estimators are grouped in Figure 11 and are presented for comparison to results from the Ohio tributaries. Individual years for each of the Ohio tributaries are grouped and presented in Figures 12 - 14. Results from semi - monthly (a) and event (b) sampling are presented in each figure.

4.2 Test Case Comparisons

Comparisons of the overall levels of estimate MSE indicate that estimator performance is much different among tributaries. RMSE's range from 5 to 20 percent in the Michigan tributaries (Figure 11). In comparison, Ohio tributary RMSE's range from 8 to 33 percent in the Maumee River, from 8 to 37 percent in the Sandusky River and from 8 to 51 percent in Hickory Creek (Figures 12 - 14). It is expected that these differences are directly related to the event responsiveness of each system.

Differences in estimate MSE are also apparent within tributary groups. Of the Michigan tributaries, the Saginaw River in 1978 had the highest MSE for every estimator and sampling scenario. The hydrograph for the Saginaw in 1978 (Figure 1) reveals one large discrete event which may have caused higher error for this test case. Reasons for differences in the Ohio tributaries are less clear. The year 1984 in Hickory Creek and the

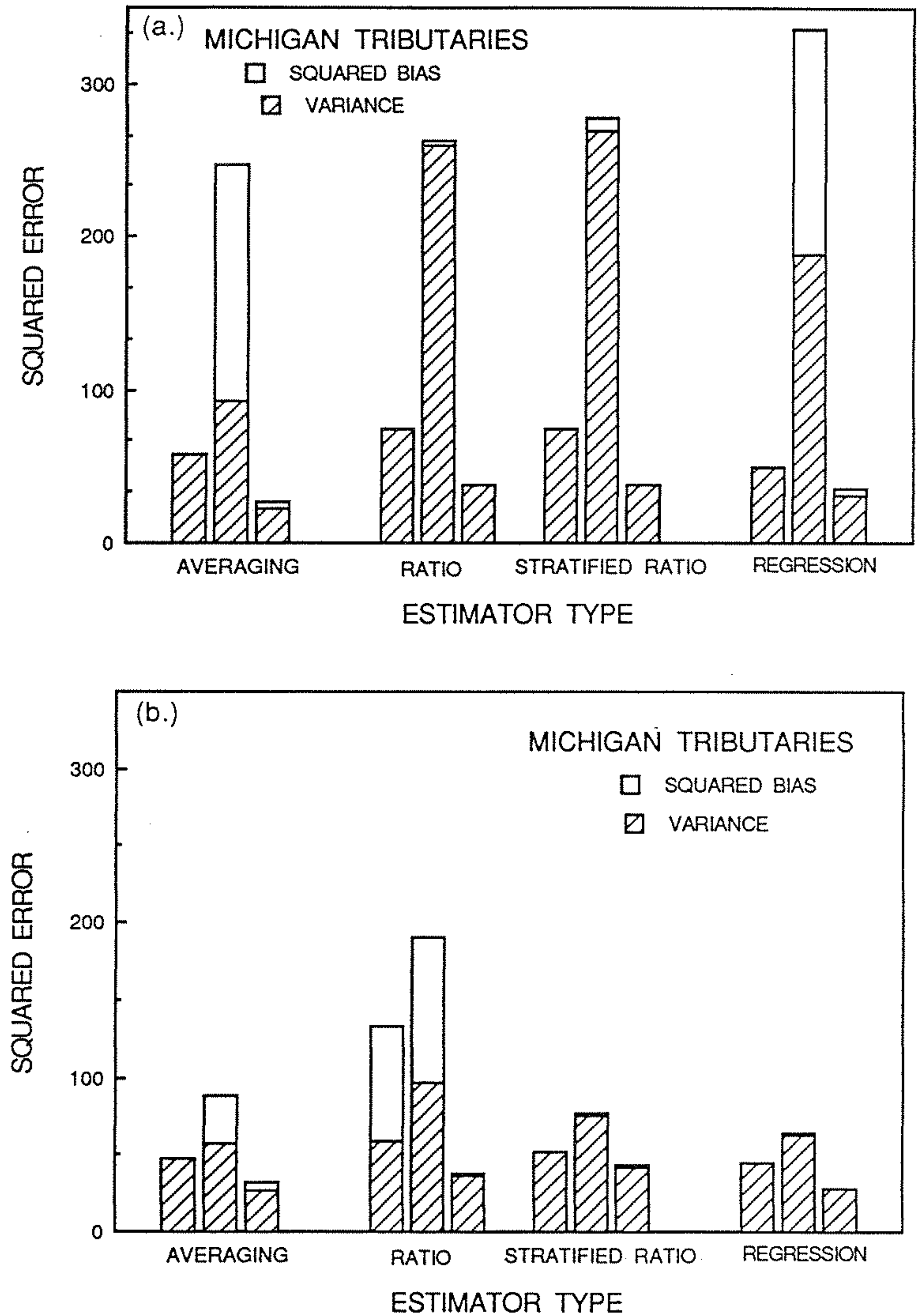

Figure 11. Summary of estimation error under systematic sampling (a.) and event sampling (b.) in the Michigan tributaries. Test cases are grouped under each estimator and are presented in the same order as Table 1. The MSE (vertical axis) is divided into squared bias (open area) and variance (hatched area).

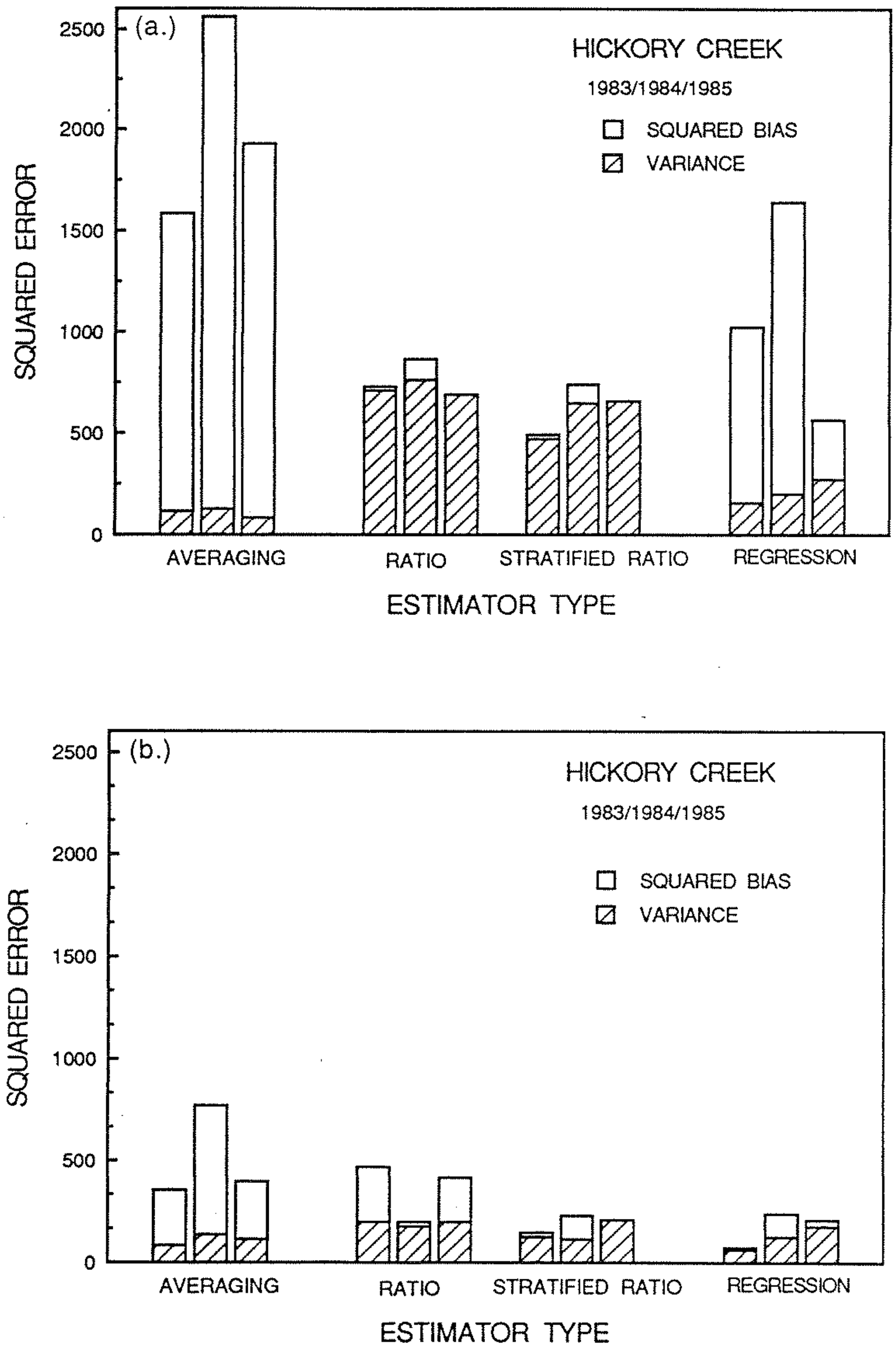

Figure 12. Summary of estimation error under systematic sampling (a.) and event sampling (b.) in Hickory Creek. Test case years are grouped under each estimator and are presented in sequential order. The MSE (vertical axis) is divided into squared bias (open area) and variance (hatched area).

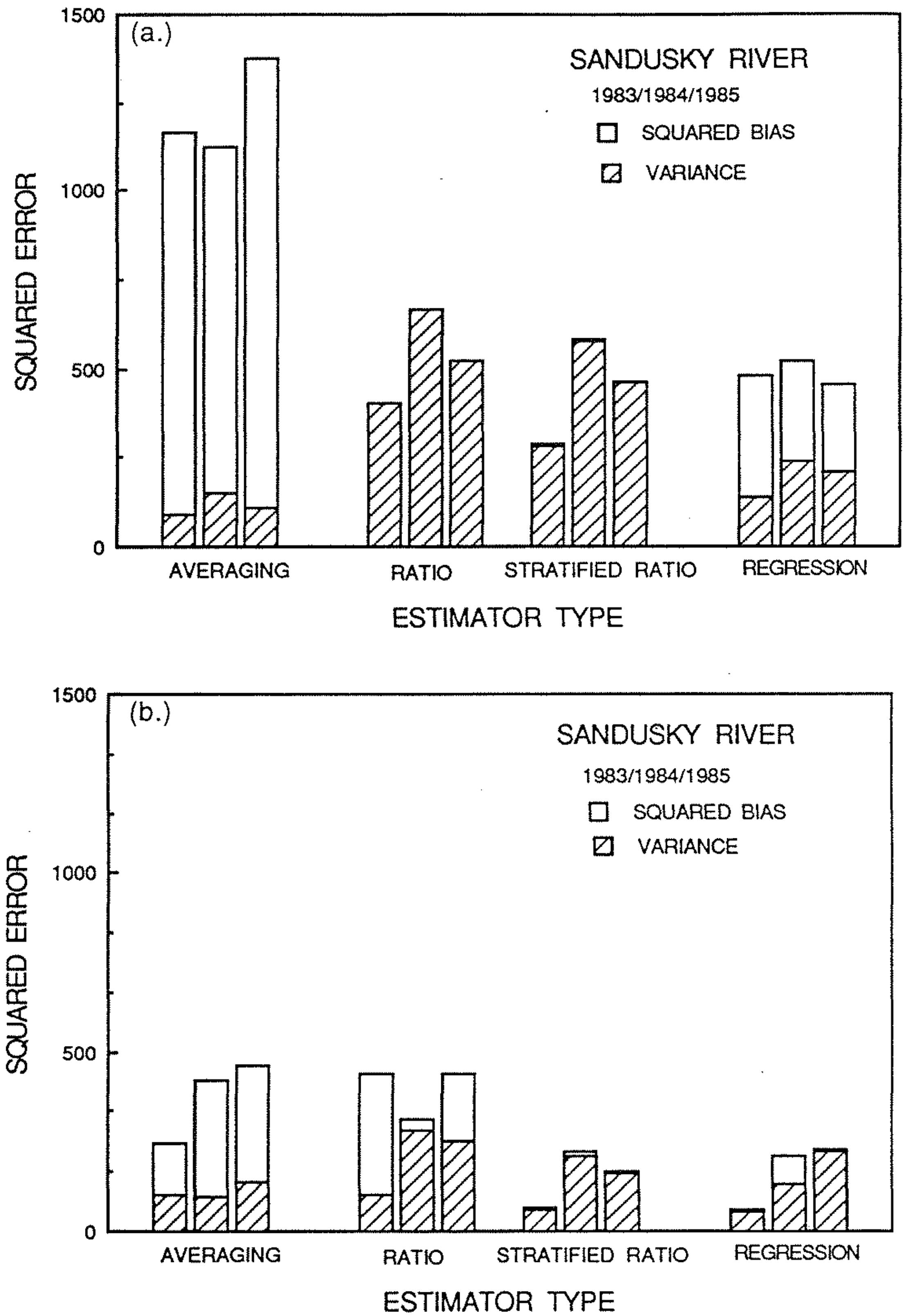

Figure 13. Summary of estimation error under systematic sampling (a.) and event sampling (b.) in the Sandusky River. Test case years are grouped under each estimator and are presented in sequential order. The MSE (vertical axis) is divided into squared bias (open area) and variance (hatched area).

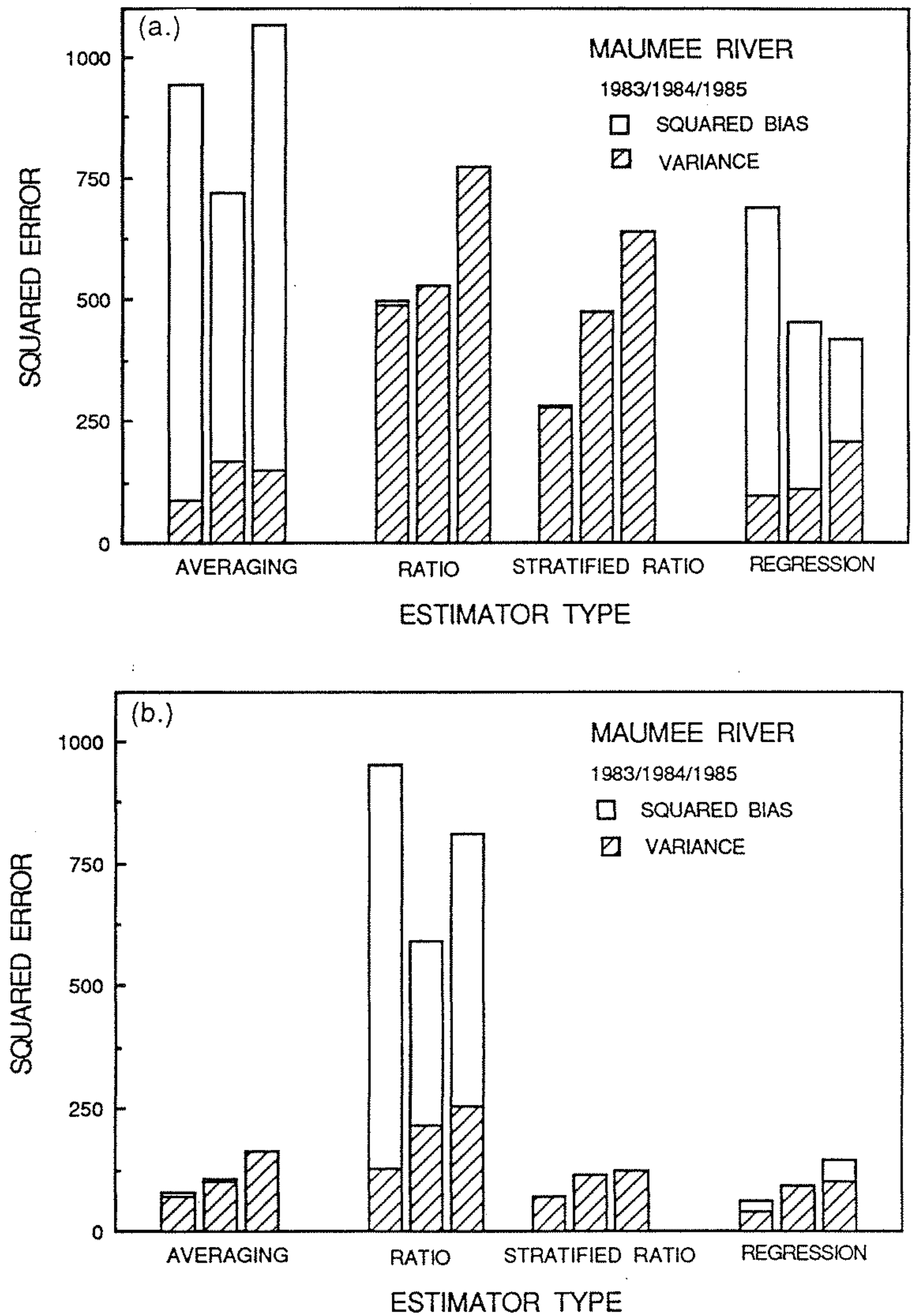

Figure 14. Summary of estimation error under systematic sampling (a.) and event sampling (b.) in the Maumee River. Test case years are grouped under each estimator and are presented in sequential order. The MSE (vertical axis) is divided into squared bias (open area) and variance (hatched area).

Sandusky River produced the greatest MSE for most estimators under systematic sampling. In both tributaries a number of discrete events occurred (Figures 2 and 3). The year 1985 in the Maumee River produced the greatest MSE for most estimators. The hydrograph in this case is characterized by a small number of large events (Figure 4).

4.3 Estimator Comparisons

No one estimator was optimal under all conditions tested. The averaging estimator provided low error estimates in a few cases, but was highly biased in others. The ratio estimator was frequently unbiased, but sometimes had high variance. The regression estimator could be highly biased, especially under systematic sampling in event responsive systems.

The averaging estimator provided low error estimates in two Michigan test cases (Grand and Saginaw, 1980). However, high bias was observed when this estimator was applied to other test cases under systematic sampling. High bias was observed whenever discrete events were present in the hydrograph. Furthermore, bias was always negative indicating that the actual load was underestimated. Bias was reduced by event sampling, but was still high relative to other estimators.

The overall MSE level of the ratio estimator was comparable to other estimators under systematic sampling. However, the error consisted of variance and the ratio estimator was virtually unbiased in all test cases. Under event sampling the overall level of estimate error was reduced. However, the ratio estimator was strongly biased unless stratified. Little difference was observed between the stratified and unstratified ratio estimators under systematic sampling.

The regression estimator (MVUE) was often highly biased when applied to event responsive test cases. Like the averaging estimator, the MVUE underestimated the actual load when applied under systematic sampling. Event sampling reduced the bias and the overall level of error. However, bias was sometimes present even under event sampling.

4.4 Comparison of Sampling Strategies

Event sampling improved load estimation in three ways. First, the overall level of error was reduced for virtually all estimators in all test cases. One exception is the unstratified ratio estimator which was highly biased under this sampling scenario. Thus the ratio estimator must be stratified to benefit from event sampling. A second benefit is that the effect of strong events is reduced. The level of error in the 1978 Saginaw River was reduced to near the level of other Michigan test cases by event sampling (Figure 11). Finally, event sampling reduced or eliminated the bias observed in the averaging estimator and MVUE under systematic sampling.

4.5 Discussion

Of the estimators considered, only the ratio estimator consistently provided unbiased estimates. The averaging and regression estimates were frequently biased and the bias appeared to be related to the occurence of discrete high flow events. The ratio estimator was more robust to the bias caused by high flow events and was virtually unbiased even for the most responsive system, Hickory Creek. The ratio estimator also provided estimate distributions that frequently had low MSE's. The fact that the ratio estimator is robust to sources of bias and often provides a low MSE indicates that it may be the most appropriate of the considered estimators for the tributary load problem.

Results of the sampling studies emphasize the value of event sampling. Even with the arbitrary 50/50 strata allocation, MSE's were substantially reduced with event sampling. It is expected that this MSE reduction can be improved upon with further research into optimum allocation strategies and this work has already been started by Richards and Holloway (1987). In addition to overall reduction in MSE, event sampling reduced the bias of the averaging and regression estimators, although some bias remained in the more responsive systems (Sandusky River and Hickory Creek). Based on the results of these studies it is apparent that some allocation of samples to events should be performed in any load estimation program. Even though the optimum allocation may be unknown, reservation of some samples specifically for high flow events can be expected to reduce load estimate error.

Estimator performance was strongly dependent upon test case characteristics. The overall RMSE ranged from 5 percent in the Saginaw in 1980 to over 50 percent in Hickory Creek during 1984. Furthermore, the level of bias in averaging and regression estimates differed strongly among tributaries. Test case characteristics that may be responsible for these differences include the nature of high flow events in the tributaries and the behavior of the contaminant in the system. Event frequency, magnitude and duration are three flow characteristics that differ among the tributary test cases. Differences in constituent behavior and flow / concentration relationship were also observed.

To efficiently make tributary loading estimates, the relative impact of each of the mentioned characteristics should be understood. The most important characteristics are not easily identified because they interact and their individual effects are difficult to isolate. Knowledge of which characteristics produce the greatest estimate error may provide a basis for sampling design and estimator choice.

The empirical studies performed have two major limitations. First, each test case is one realization of a continuous random process. Conclusions based on a small number of realizations are limited and may not be reflective of the entire process. It is also difficult to isolate the impact of potential sources of estimate error. Comparison of test cases allows inferences to be drawn. However, it does not allow definitive study of the impact of event characteristics on estimate error.

A means of avoiding the limitations of the empirical studies is to simulate data using statistical models. Data simulation allows the evaluation of sampling scenarios and estimation error under the broadest possible conditions. By systematically varying the level of a particular characteristic (e.g. - event frequency) the sensitivity of estimate error to the characteristic can be assessed. In this way, the most important characteristics can be determined and used as a basis for the design of sampling programs for load estimation.

5. DATA SIMULATION

Work has been performed to design an approach for simulation of daily flows. Two modeling approaches are being evaluated including a Multicomponent model (Vandeweile and Dom, 1989) and a Threshold ARMAX model (Tong et al., 1985). These models are being evaluated for their ability to simulate tributary flow over the range of tributary types described by Richards (1988). Review of literature on flow simulation and descriptions of the two modeling approaches follow.

5.1 Literature Review

A great deal of research has been performed on methods for simulation of river flows (Lawrence and Kottegoda, 1977). The impetus of this work has been the study of extremes for reservoir design or for flood or drought occurence. Most of the models used are statistical time series models. Some of these include

1.) Spectral Analysis

2.) ARIMA Models

3.) Box - Jenkins Seasonal Models

4.) Fractional Gaussian Noise Models

5.) Multisite Models

6.) Disaggregation Models.

Many of these models assume stationarity and are primarily applied to mean annual flows. Non - stationary or seasonal models have been devised for the simulation of monthly mean flows. However, simulation of daily flows is much more complicated because of the rapid ascensions and slow recessions of individual events (Kottegoda, 1980). Consequently, much less work has been published on daily flow simulation models.

ARIMA models can be adapted for periodic data. Using the notation of Box and Jenkins (1976), the seasonal ARMA(p,q) model can be expressed as

$$\phi_p(B) \cdot \Phi_p(B^s)\ y_t = \theta_q(B) . \Theta_p(B^s)\ a_t$$

where

ϕ_p, Φ_p, θ_q, Θ_p - coefficient matrices

B - backward shift operator

s - degree of periodicity

y_t - variable of interest

a_t - random component.

ARIMA models are parsimonious relative to other seasonal models (disaggregation) and this may enhance accurate reproduction of flow characteristics (Stedinger et al., 1985). However, ARIMA models are primarily used for forecasting and are cumbersome for use in simulation. McMichael and Hunter (1972) compared this approach with the use of a deterministic - stochastic model (periodic function with autoregressive component) for simulating Ohio River flows and temperatures. Both models were considered equally parsimonious. However, the deterministic - stochastic model more closely approximated the two time series.

A second method for simulating seasonal data is by using disaggregation models. This approach was originally proposed by Valencia and Schaake (1973) and uses annual flow values as input to generate seasonal data. The general form for a single site Markovian model is

$$X_{y\,(nT \times 1)} = A_{(nT \times N)}\, Z_{y\,(N \times 1)} + B_{(nT \times nT)}\, V_{y\,(nT \times 1)}$$

where

X_y - vector of generated flows

Z_y - vector of annual transformed normally distributed flows

V_y - vector of standard normal deviates

A, B - coefficient matrices

n - number of years to be simulated

T - number of within year data to be simulated

N - number of actual annual means.

This model is adaptable for multiple sites and multiple lags (Loucks et al., 1981);

however, discontinuities can sometimes occur between periods.

Much less research has been performed on daily flow simulation models. Weiss (1977) proposed a "Shot Noise" model which consists of a series of events that occur randomly, have random magnitude and recede at a fixed rate. Koch (1985) derived statistical moments of a simplified physically based streamflow model. Prediction using this model was stated to be limited by knowledge of spatial variability and initial values of parameters. Ozaki (1985) described the use of storage models driven by randomly generated rainfall sequences for streamflow simulation. Tong et al. (1985) proposed the use of a threshold ARMAX model that can account for seasonal shifts in rainfall runoff relationships due to freeze / thaw effects. Vandewiele and Dom (1989) proposed a "Multicomponent" model which treats event initiations, event recessions and baseflow as separate processes that can be combined to simulate daily flow sequences. Little work has been performed to compare daily flow models for their ability to reproduce actual flow characteristics.

5.2 Flow Simulation Models

5.2.1 Multicomponent Model

The multicomponent model decomposes tributary flow rates into a number of processes that occur at different frequencies. These include long term shifts in annual mean flow rate, seasonal periodic shifts in baseflow and short term event occurences. This approach was originally proposed by Fiering (1967) and has been used for simulation of daily flow (McMichael and Hunter, 1972) and daily water quality (Sanders and Adrian, 1978). Our model is a modification of the work of these authors that allows the realistic simulation of events.

The overall form of the model is represented as the sum of individual processes.

$$q_{yt} = \mu_y + Se_t + Ei_{yt} + (1 - W)\, Er_{yt} + W\, Ac_{yt} + \varepsilon_{yt}$$

where

q_{yt}= log transformed flow

μ_y = annual log mean

Se_t = periodic seasonal term

Ei_{yt} = random event initiation

Er_{yt} = event recession

W = weighting function

Ac_{yt} = autocorrelated process

ε_{yt} = random residuals.

The log transform of flow values was used since it reduces the skew and facilitates the fitting process. The annual mean was incorporated to account for small year to year climatic variations. Seasonal periodicities were modeled using annual and semi - annual harmonics which were identified as the dominant periodic frequencies by spectral analysis.

Strong events were apparent in some tributaries and not in others. To allow the occurence of events as a separate process, a weighting function was introduced. This function was designed to weight event recessions more heavily during high flow conditions and autocorrelated random variations in the log transformed flows during non - event periods. In this way non - reversibilities in the random process (event recession) could be modeled. In addition both non - responsive and responsive systems could be modeled purely as a function of parameter values.

Events are modeled using the "Shot Noise" approach of Weiss (1977). Event initiations occur as instantaneous increases in the daily mean flow rate. Initiations or "shots" are randomly generated with exponentially distributed arrival times and magnitudes. After the initiation of an event the flow rate recedes exponentially at a rate determined by the fitting procedure.

The model is fitted using non - linear least squares with the Gauss - Newton algorithm. This is based on a truncated Taylor Series and can be expressed as

$$Q^* = Q_a - \hat{Q}_1 + X_1 \beta_1 = X_1 \beta_2 + \varepsilon^*$$

where

Q_a = actual log transformed flow matrix

$\hat{Q}_1$ = estimated log flow matrix at first iteration

$\mathbf{X}_1$ = derivative matrix evaluated at first iteration

$\mathbf{\beta}_1$ = parameter array at first iteration

or

$$Q^* = X_1\ \beta_2 + e^*.$$

Each year is treated as a discrete realization of the long term process and the matrices are set up as

$$\begin{pmatrix} Q^*_{i\,1} \\ Q^*_{i\,2} \\ \vdots \\ Q^*_{i\,N} \end{pmatrix} = \begin{pmatrix} X_{i\,1} \\ X_{i\,2} \\ \vdots \\ X_{i\,N} \end{pmatrix} (\beta) + \begin{pmatrix} e_{i\,1} \\ e_{i\,2} \\ \vdots \\ e_{i\,N} \end{pmatrix}$$

where

Q^*_{ij} = transformed flow at i^{th} iteration in year j

$\mathbf{X}_{ij}$ = derivative matrix at iteration i and year j

$\mathbf{\beta}$ = parameter matrix

ε_{ij} = error term at iteration i and year j.

The derivative matrix can be specified as

$$\mathbf{X} = \begin{pmatrix} 1 & 0 & \cdots & 0 & \cdots & \mathbf{d}_{ijk} & \cdots & \mathbf{d}_{ijk} \\ 0 & 1 & \cdots & 0 & \cdots & \mathbf{d}_{ijk} & \cdots & \mathbf{d}_{ijk} \\ \vdots & \vdots & & \vdots & & \vdots & & \vdots \\ 0 & 0 & \cdots & 1 & \cdots & \mathbf{d}_{ijk} & \cdots & \mathbf{d}_{ijk} \end{pmatrix}$$

where $\mathbf{d}_{ijk}$ is the derivative array at iteration i, year j and with respect to parameter k. The ordinary least squares solution to the system of equations can be expressed as

$$\hat{\beta} = (X'X)^{-1} X Q^{*}$$

A more efficient form of this equation is the Generalized Least Squares (GLS) form:

$$\hat{\beta} = (X' \quad \hat{\Omega}^{-1} \quad X)^{-1} X' \quad \hat{\Omega}^{-1} \quad Q^{*}$$

where $\hat{\Omega}$ is a covariance matrix of the residuals. The GLS form of the equation improves the efficiency in the estimation by taking advantage of any covariance in the residuals between years. It also helps to insure stationary residuals by weighting the function by the variance within years.

Fitting is performed by iteratively solving the linear system of equations and updating parameter values. Iteration begins using initial estimates of parameter values. It continues until stable parameter values are found and the objective function is minimized.

The Multicomponent model offers the advantage of allowing simulation based purely on the characteristics of flow records. However, it also has two major limitations. First, event initiations cannot be fitted as part of the overall model and must be defined arbitrarily. Definition of events is clear in responsive systems, but is much less clear in stable systems. A second limitation of the model is that its use in sensitivity analysis is complicated by the fact that the individual processes are interrelated. Testing the sensitivity of error to individual processes may not be realistic because of interrelationships.

5.2.2 Threshold Model

A second model being evaluated is called a Threshold Time Series (Tong et al., 1985) The model is a subset of the ARMAX class of time series models and uses rainfall and temperature as independent variables. It offers the advantage of being able to compensate for non - linearities caused by freeze/thaw flow differences. The model is piecewise linear and can be expressed as

$$Q(t) = \sum_{i=1}^{n} D_i \left[A + \sum_{j=1}^{M_1} B_j\, Q(t-j) + \sum_{k=0}^{M_2} C_k\, P(t-k) + \sum_{l=0}^{M_3} E_l\, T(t-l) \right]_i + \varepsilon_t$$

where

$Q(t)$ = flow at time t

$P(t)$ = precipitation at time t

$T(t)$ = temperature at time t

D_i = (0,1) dummy variable defined by value of T

A, B, C, E = model coefficients

n = number of segments.

To implement the model threshold locations must be found based on non-linearities in the relationship between flow and temperature. Tong et al. (1985) demonstrated the performance of this model for two tributaries in Iceland. Evaluations are now being performed to determine if the model will be adequate for simulation of riverflow in Great Lakes tributaries.

Sensitivity analysis using the Threshold model can be performed based on random variations in precipitation and temperature. For example, since the frequency and magnitude of rainfall events determine flow variability, sensitivity to these factors is analogous to sensitivity to flow variability. Variations in precipitation and temperature can be input to the model either by using actual data or by devising models for the forcing functions. Current studies are underway to evaluate these two alternatives.

One of the greatest drawbacks of the threshold model as described by Tong et al. (1985) is that the model is not easily calibrated. The authors do not describe their fitting routine in detail. However, parameter values and threshold locations appear to be estimated by a trial and error minimization of the Normalized Akaike Information Criterion (NAIC). This procedure could be improved by the methods of Marsh (1988). This approach entails rough estimation of threshold locations and parameter values using stepwise regression. A Gauss-Newton iteration method is then invoked to obtain simultaneous least squares improvements on parameter and threshold location estimates.

5. CONCLUSIONS AND RECOMMENDATIONS

The following major conclusions can be drawn based on the results of this research:

1. No single estimation approach was found to be optimal under all conditions tested. However, the ratio estimator is consistently unbiased and frequently provides an estimate with low MSE.

2. Although the event sampling performed in this study may not be an optimal design, it is apparent that some sample allocation to high flows can provide substantial benefits. Among these benefits is an overall reduction in MSE, a reduction in estimate bias and a reduction in the impact of discrete events.

3. Stratification of the Ratio estimator is essential to maintain its accuracy under event sampling.

4. Strong differences in estimation error are apparent among the test cases considered. Based on the results of this study it is hypothesized that differences in event frequency, magnitude and duration among tributaries are primarily responsible for this effect. The particular flow - concentration relationship in the tributary is probably the other major factor. Studies are currently underway to evaluate these hypotheses.

The following recommendations are made for future research:

1. The hypotheses concerning the causes of loading estimate error should be evaluated. Sensitivity analyses should identify the most important tributary characteristics. These characteristics may then provide a basis for the design of sampling programs and lead to the goal of finding an overall design scheme to be used in load estimation.

2. Further research should be performed to continue the work of Richards and Holloway (1987) and to investigate different design schemes for load estimation sampling programs. Design criteria should be found for the number of flow strata to be used and sample allocation within each strata. Furthermore, mechanisms need to be found

that will identify the optimal time during which event samples should be collected.

3. Research should be continued to find appropriate models for the simulation of loading data. These models should be flexible enough to allow the simulation of flow and concentration data from a variety of tributary types.

6. NUMBER AND DISCIPLINE OF STUDENTS ASSISTING ON THE PROJECT

One graduate student, Mr. Stephen D. Preston, assisted on the project on a full time basis. One undergraduate student, Ms. Levia Stein, assisted on the project during the summer 1988. Ms. Stein was supported through a National Science Foundation grant to the Department of Civil Engineering as part of a program on Undergraduate Research Experiences. The major discipline for both students is Environmental Engineering.

7. EMPLOYMENT STATUS OF STUDENTS ASSISTING ON PROJECT

Mr. Stephen D. Preston is presently a full time graduate student in the Department of Civil Engineering. He is expected to complete requirements for the doctoral degree in December 1989.

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